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An ab initio Study of Atomic Hydrogen Sorption on the Zigzag Edge of Pristine Bilayer Graphene

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Abstract: We studied the sorption mechanism of atomic hydrogen on the zigzag edge of pristine bilayer graphene (BLG) as groundwork effort in the realization of the material's utilization as the substrate in a hydrogen storage system. Using density functional theory, we performed total energy calculations, using pseudopotentials obtained from projector augmented wave (PAW) method. The Kohn-Sham equations were solved using plane waves with kinetic energies of 400 eV. The surface Brillouin zone integration was performed using the special-point sampling technique of Monkhorst and Pack (with 4×4×1 sampling meshes). For the exchange correlation energy, we adopted the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional. Each layer in the slab model we used in the calculations consisted of 28 sp^2-bonded carbon atoms with in-plane carbon-carbon distance of 1.42 Å and out-of-plane equilibrium stacking distance of 3.5 Å. Results revealed at least two non-activated reaction paths (paths of least potential) on pristine bilayer graphene which confirmed the possibility of absorbing H in between the carbon layers. Also, the strong H trap near the surface C atoms conveyed the strong tendency of C atoms to form sp^2p_z hybridization in the initial stage of H adsorption. The results suggest the possible utility of the zigzag edge as a reaction channel to carry out the sorption process.

Key Words: density functional theory; hydrogen; graphene; hydrogen storage; hydrogen fuel